

N,N-Diethylaniline
91-66-7 | DTXSID8021800

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 5.33

Global applicability domain: Inside

Local applicability domain index: 9.36e-01

Confidence level: 7.30e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,4-Dibromobenzene</div> <div>Measured: 5.21</div> <div>Predicted: 5.09</div>	<div>Image not found</div> <div>Hexamethylbenzene</div> <div>Measured: 6.31</div> <div>Predicted: 5.75</div>	<div>Image not found</div> <div>Naphthalene</div> <div>Measured: 5.19</div> <div>Predicted: 5.07</div>
<div>Image not found</div> <div>1,3,5-Trichlorobenzene</div> <div>Measured: 4.85</div> <div>Predicted: 5.06</div>	<div>Image not found</div> <div>1,2,4-Trichlorobenzene</div> <div>Measured: 4.95</div> <div>Predicted: 5.06</div>	